entre 2,104 et 3,332 Å. La plus courte distance (2,104 Å) est celle que l'on observe habituellement dans les polysulfures (Teske, 1974; Leclerc & Kabré, 1975); elle montre l'existence d'une liaison covalente entre atomes de soufre, c'est-à-dire d'un groupement disulfure (S–S).

Comme l'a indiqué Flahaut (1976) pour les composés des terres rares contenant du soufre et un second non-métal, on est en présence d'un feuillet plan cationique $(LaS)_n^{n+}$ associé à un plan polyatomique $(S–S)_n^{2n-}$. La formule chimique du polysulfure de lanthane peut donc être écrite: $(LaS)(S–S)_{0,5}$.

Cette disposition en feuillets de pyramides [Ln$_5$S] a déjà été décrite pour l'arséniosulfure de cérium, (CeS)As, par Sfez & Adolphe (1972) et est caractéristique du type anti-Fe$_2$As(C38). On peut, comme le montre la Fig. 1, mettre en évidence dans la maille cristalline du polysulfure de lanthane LaS$_2$, la présence d'un motif type anti-Fe$_2$As légèrement déformé.

Il est intéressant de remarquer que le polysulfure d'ytterbium YbS$_2$, décrit par Teske (1974), possède une structure formée par l'association de tétraèdres [Yb$_4$S], tous les atomes de soufre étant équivalents et engagés dans une liaison disulfure (distance S–S égale à 2,11 Å); sa formule chimique doit donc s'écrire Yb(S–S), ce qui implique que l'atome d'ytterbium possède la valence

2. Par contre dans les structures en feuillets à deux anions MXY, comme (CeS)As et $(LaS)(S–S)_{0,5}$, la terre rare possède la valence 3.

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The Crystal and Molecular Structures of Magnesium Di-o-phthalatocuprate(II) Dihydrate and Strontium Di-o-phthalatocuprate(II) Trihydrate

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(I) MgCu(C$_8$H$_4$O$_4$)$_2$.2H$_2$O: orthorhombic $P2_12_12$; $a = 6.551$ (7), $b = 20.589$ (10), $c = 6.832$ (8) Å, $Z = 2$. (II) SrCu(C$_8$H$_4$O$_4$)$_2$.3H$_2$O: monoclinic $C2/c$; $a = 22.144$ (18), $b = 9.122$ (9), $c = 9.083$ (8) Å, $\beta = 103.6$ (1)°, $Z = 4$. The structures, determined from diffractometer data by Patterson and Fourier methods, were refined by least squares to $R = 3.7\%$ for both compounds. Both structures consist of o-phthalatocuprate(II) complexes, joined in linear polymeric chains by bridging o-phthalate anions, of alkaline-earth cations and of water molecules. In (I) Cu is square planar, coordinated by four O atoms from four o-phthalate groups. In (II) Cu is octahedral, coordinated by six O atoms from four o-phthalate anions acting as tridentate (chelating and bridging) ligands. Coordination of Mg is octahedral and involves two O atoms from two o-phthalate anions belonging to adjacent chains and four water molecules. The Mg–O bonds are in the range 2.031–2.070 Å. Sr is surrounded by six O atoms from four o-phthalate groups belonging to the same chain and by three water molecules, so that the coordination polyhedron can be described as a distorted trigonal prism with lateral centred faces. The Sr–O bond distances are in the range 2.549–2.773 Å.

Introduction

The o-phthalate (pht) anion, when coordinating to Cu^{II} atoms through two O atoms from the two carboxylate groups, can bridge metal atoms giving rise to polymeric chains (Cingi, Guastini, Musatti & Nardelli, 1970; Cingi, Lanfredi, Tiripicchio & Camellini, 1977, 1978b) or chelate a metal atom in such a way as

to form monomeric complexes (Cingi, Lanfredi, Tiripicchio & Camellini, 1978c). When the pht anion behaves as a tridentate ligand, coordinating to adjacent Cu through three O atoms, layers of Cu complexes are present (Cingi, Lanfredi, Tiripicchio & Camellini, 1978a; Prout, Carruthers & Rossotti, 1971). In both compounds described in the present paper, the pht anion acts as a tridentate ligand but in a way different from that already observed: in the Mg compound (I) pht bridges adjacent Cu atoms in polymeric chains joined in layers by the interaction of a third O atom of the pht anion with Mg; in the Sr compound (II), pht behaves as a chelating and bridging ligand according to the scheme below.
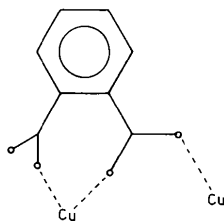
Experimental

The compounds were prepared by slow evaporation at room temperature of aqueous solutions obtained by dissolving Cu^{II} carbonate hydroxide and Mg or Sr carbonate in a warm solution of phthalic acid.

Table 1. *Fractional atomic coordinates for* (I) ($\times 10^4$ *for* Cu, Mg, O, C *atoms*; $\times 10^3$ *for* H *atoms*) *with e.s.d.'s*

	x	y	z
Cu	0	0	2748 (1)
Mg	5000	0	8909 (4)
O(1)	−173 (10)	716 (2)	10925 (5)
O(2)	2179 (6)	406 (2)	8760 (6)
O(3)	−237 (10)	652 (2)	4797 (5)
O(4)	3015 (7)	872 (2)	4213 (7)
O_w(1)	6089 (9)	663 (3)	6921 (8)
O_w(2)	5709 (8)	641 (3)	11142 (8)
C(1)	789 (10)	1455 (3)	8469 (9)
C(2)	1189 (10)	1539 (3)	6460 (9)
C(3)	1265 (12)	2158 (3)	5702 (11)
C(4)	967 (13)	2696 (3)	6877 (11)
C(5)	504 (11)	2613 (3)	8835 (10)
C(6)	421 (11)	1995 (3)	9614 (9)
C(7)	984 (10)	799 (3)	9432 (9)
C(8)	1365 (11)	975 (3)	5058 (8)
H(11)	521 (13)	61 (3)	583 (11)
H(21)	709 (14)	77 (4)	637 (13)
H(12)	501 (12)	82 (3)	1222 (8)
H(22)	699 (13)	74 (4)	1136 (11)
H(3)	181 (11)	220 (3)	424 (11)
H(4)	109 (9)	314 (3)	619 (8)
H(5)	−17 (14)	298 (3)	960 (9)
H(6)	−15 (14)	192 (3)	1100 (9)

Table 2. *Fractional atomic coordinates for* (II) ($\times 10^4$ *for* Cu, Sr, O, C *atoms*; $\times 10^3$ *for* H *atoms*) *with e.s.d.'s*

|	x	y	z
Cu	0	0	0
Sr	0	−3141 (1)	2500
O(1)	403 (2)	1926 (5)	361 (5)
O(2)	1004 (2)	3585 (6)	−309 (5)
O(3)	658 (2)	−782 (5)	2364 (5)
O(4)	655 (2)	885 (5)	4149 (5)
O_w(1)	0	4065 (8)	2500
O_w(2)	786 (2)	−3637 (6)	852 (6)
C(1)	1493 (3)	1983 (7)	1648 (7)
C(2)	1455 (3)	1033 (8)	2843 (7)
C(3)	1994 (3)	664 (9)	3899 (8)
C(4)	2570 (3)	1186 (10)	3756 (9)
C(5)	2609 (3)	2088 (9)	2570 (9)
C(6)	2077 (3)	2488 (9)	1532 (8)
C(7)	936 (3)	2511 (7)	478 (7)
C(8)	869 (3)	308 (7)	3088 (7)
H(1)	200 (3)	6 (8)	482 (7)
H(2)	299 (4)	72 (9)	438 (9)
H(3)	299 (3)	235 (8)	240 (8)
H(4)	212 (3)	318 (8)	74 (7)
H(5)	11 (3)	352 (8)	194 (7)
H(6)	92 (4)	−438 (9)	38 (9)
H(7)	78 (4)	−290 (10)	42 (9)
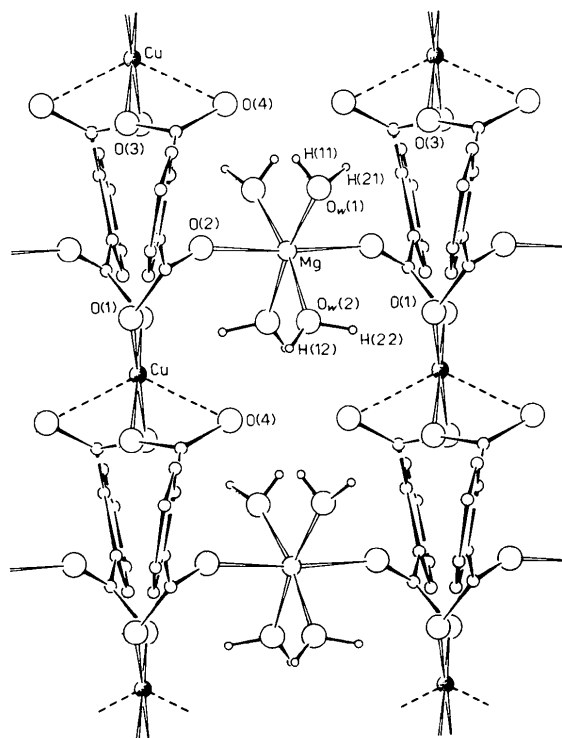
Fig. 1. Projection of the structure of the Mg compound along [010].

Crystal data

(I) $C_{16}H_{12}CuMgO_{10}$, $M_r = 452 \cdot 1$, orthorhombic, $a = 6 \cdot 551$ (7), $b = 20 \cdot 589$ (10), $c = 6 \cdot 832$ (8) Å, $V = 921$ (2) Å^3, $D_c = 1 \cdot 63$ g cm^{-3}, $Z = 2$, $F(000) = 458$; Mo $K\alpha$ radiation, $\lambda = 0 \cdot 71069$ Å, μ(Mo $K\alpha$) = 12·70 cm^{-1}. Space group $P2_12_12$ from systematic absences and from structure determination.

(II) $C_{16}H_{14}CuO_{11}Sr$, $M_r = 533 \cdot 4$, monoclinic, $a = 22 \cdot 144$ (18), $b = 9 \cdot 122$ (9), $c = 9 \cdot 083$ (8) Å, $\beta = 103 \cdot 6$ (1)°, $V = 1783$ (3) Å^3, $D_c = 1 \cdot 99$ g cm^{-3}, $Z = 4$, $F(000) = 1060$, Mo $K\alpha$ radiation, $\lambda = 0 \cdot 71069$ Å, μ(Mo $K\alpha$) = 60·11 cm^{-1}. Space group $C2/c$ from systematic absences and from structure determination. Unit-cell parameters were determined from rotation and Weissenberg photographs and refined from diffractometer data.

Intensity data

Intensities for compounds (I) and (II) were collected on a Siemens AED single-crystal diffractometer with Zr-filtered Mo $K\alpha$ radiation and the $\omega - 2\theta$ scan technique. Prismatic crystals of dimensions $ca\ 0 \cdot 180 \times 0 \cdot 220 \times 0 \cdot 310$ mm (I) and $0 \cdot 045 \times 0 \cdot 095 \times 0 \cdot 300$ mm (II) were aligned with **a** (I) and **c** (II) along the φ axis of the diffractometer and all the reflexions with $6 < 2\theta < 50°$ (I) and $2\theta < 50°$ (II) were measured. Of 982 (I) and 1567 (II) independent reflexions, 876 (I) and 1078 (II) having $I > 2\sigma(I)$ were used in structure determinations. Corrections for Lorentz and polarization factors were made but not for absorption. The first absolute scaling and the overall isotropic temperature factor were obtained by Wilson's (1942) method.

Structure determination and refinement

The structures were solved by Patterson and Fourier methods and refined by block-diagonal (II) and full-matrix (I) least squares, at first with isotropic, then with anisotropic thermal parameters. The H atoms were located directly from a ΔF synthesis and refined by least squares with isotropic thermal parameters. Unit weights were used in all stages of the refinement by analysing the variations of $|\Delta F|$ as a function of $|F|$. The final conventional R index was 0·037 for both compounds (observed reflexions only). Atomic scattering factors from Cromer & Mann (1968) were used for non-hydrogen atoms and those of Stewart, Davidson & Simpson (1965) for H. Final atomic coordinates are given in Table 1 for (I), and Table 2 for (II).*
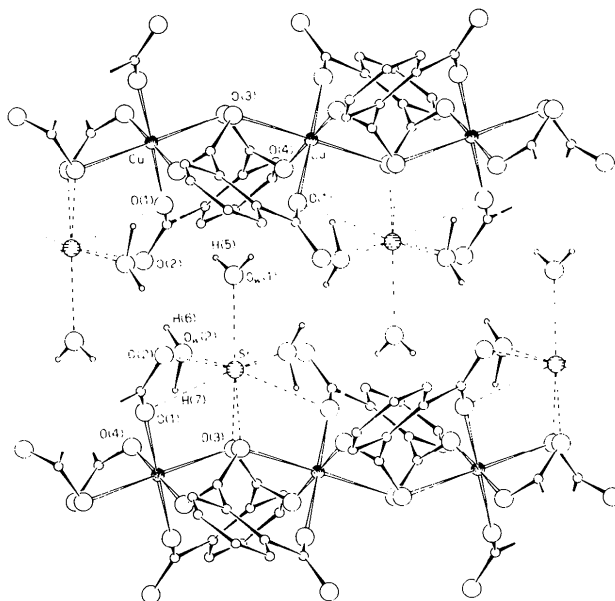

Fig. 2. Projection of the structure of the Sr compound along [100].
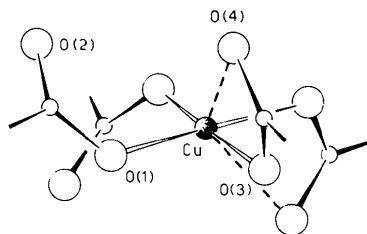

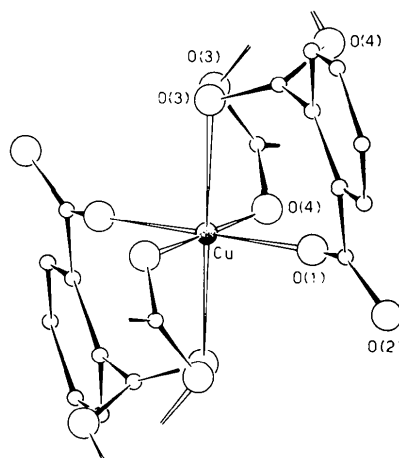Fig. 3. Coordination around the Cu atom in the Mg compound.

Fig. 4. Coordination around the Cu atom in the Sr compound.

Table 3. *Bond distances* (Å) *and angles* (°) *in the magnesium compound*

(a) In the coordination polyhedron

Cu—O(3)	1·946 (4)	Cu—O(4)	2·851 (5)
Cu—O(1ⁱ)	1·933 (4)		

O(3)—Cu—O(1ⁱ)	86·1 (1)	O(4)—Cu—O(3ⁱⁱⁱ)	97·3 (2)
O(3)—Cu—O(4)	50·8 (2)	O(3)—Cu—O(1ⁱⁱ)	173·9 (2)
O(4)—Cu—O(1ⁱ)	77·7 (2)	O(1ⁱ)—Cu—O(1ⁱⁱ)	99·8 (2)
O(4)—Cu—O(1ⁱⁱ)	131·8 (2)	O(3)—Cu—O(3ⁱⁱⁱ)	88·0 (2)
O(4)—Cu—O(4ⁱⁱⁱ)	138·9 (2)		

(b) In the phthalate anion

C(1)—C(2)	1·408 (9)	C(1)—C(7)	1·508 (9)
C(2)—C(3)	1·377 (9)	C(7)—O(1)	1·282 (8)
C(3)—C(4)	1·382 (10)	C(7)—O(2)	1·216 (8)
C(4)—C(5)	1·382 (10)	C(2)—C(8)	1·510 (9)
C(5)—C(6)	1·380 (9)	C(8)—O(3)	1·255 (9)
C(1)—C(6)	1·381 (9)	C(8)—O(4)	1·244 (8)
C(3)—H(3)	1·06 (8)	C(5)—H(5)	1·02 (7)
C(4)—H(4)	1·03 (6)	C(6)—H(6)	1·03 (7)

C(2)—C(1)—C(6)	119·1 (6)	C(4)—C(5)—C(6)	119·7 (6)
C(2)—C(1)—C(7)	121·3 (6)	C(5)—C(6)—C(1)	121·1 (6)
C(6)—C(1)—C(7)	119·3 (6)	C(1)—C(7)—O(1)	114·6 (5)
C(1)—C(2)—C(3)	119·2 (6)	C(1)—C(7)—O(2)	119·1 (6)
C(1)—C(2)—C(8)	122·6 (5)	O(1)—C(7)—O(2)	126·3 (6)
C(3)—C(2)—C(8)	118·1 (6)	C(2)—C(8)—O(3)	115·7 (6)
C(2)—C(3)—C(4)	121·2 (7)	C(2)—C(8)—O(4)	119·5 (6)
C(3)—C(4)—C(5)	119·6 (6)	O(3)—C(8)—O(4)	124·8 (6)
C(2)—C(3)—H(3)	116 (3)	C(4)—C(5)—H(5)	120 (3)
C(4)—C(3)—H(3)	122 (3)	C(6)—C(5)—H(5)	118 (4)
C(3)—C(4)—H(4)	116 (3)	C(5)—C(6)—H(6)	120 (4)
C(5)—C(4)—H(4)	125 (3)	C(1)—C(6)—H(6)	118 (3)

(c) Around the magnesium cation

Mg—O(2)	2·031 (5)	Mg—O_w(2)	2·070 (6)
Mg—O_w(1)	2·054 (6)		

O(2)—Mg—O_w(1)	90·5 (2)	O_w(1)—Mg—O_w(2)	89·2 (2)
O(2)—Mg—O_w(2)	88·8 (2)	O_w(1)—Mg—O_w(1ⁱᵛ)	97·2 (3)
O(2)—Mg—O(2ⁱᵛ)	174·3 (2)	O_w(1)—Mg—O_w(2ⁱᵛ)	171·6 (2)
O(2)—Mg—O_w(1ⁱᵛ)	85·7 (2)	O_w(2)—Mg—O_w(2ⁱᵛ)	85·1 (3)
O(2)—Mg—O(2ⁱᵛ)	95·5 (2)		

(d) In the water molecules

O_w(1)—H(11)	0·95 (8)	O_w(2)—H(12)	0·94 (6)
O_w(1)—H(21)	0·79 (9)	O_w(2)—H(22)	0·88 (8)
H(11)—O_w(1)—H(21)	99 (8)	H(12)—O_w(2)—H(22)	104 (7)

(e) Hydrogen bonds

O_w(1)—H(11)···O(4)	2·768 (8)	O_w(1)—H(11)—O(4)	152 (6)
H(11)···O(4)	1·89 (8)	H(11)—O_w(1)—O(4)	19 (4)
O_w(1)—H(21)···O(3ᵛ)	2·811 (9)	O_w(1)—H(21)—O(3ᵛ)	158 (8)
H(21)···O(3ᵛ)	2·07 (9)	H(21)—O_w(1)—O(3ᵛ)	16 (6)
O_w(2)—H(12)···O(4ᵛⁱ)	2·783 (8)	O_w(2)—H(12)—O(4ᵛⁱ)	157 (6)
H(12)···O(4ᵛⁱ)	1·89 (7)	H(12)—O_w(2)—O(4ᵛⁱ)	16 (4)
O_w(2)—H(22)···O(1ᵛ)	2·706 (9)	O_w(2)—H(22)—O(1ᵛ)	156 (7)
H(22)···O(1ᵛ)	1·88 (9)	H(22)—O_w(2)—O(1ᵛ)	16 (5)

Asymmetric units

(i)	x, y, z − 1	(iv)	−x + 1, −y, z
(ii)	−x, −y, z − 1	(v)	1 + x, y, z
(iii)	−x, −y, z	(vi)	x, y, 1 + z

Table 4. *Bond distances* (Å) *and angles* (°) *in the strontium compound*

(a) In the coordination polyhedron

Cu—O(1)	1·963 (5)	Cu—O(3)	2·402 (5)
Cu—O(4ⁱ)	1·970 (6)		

O(1)—Cu—O(4ⁱ)	94·9 (3)	O(3)—Cu—O(4ⁱ)	83·2 (2)
O(1)—Cu—O(4ⁱⁱ)	85·2 (2)	O(3)—Cu—O(4ⁱⁱ)	96·8 (2)
O(3)—Cu—O(1)	87·7 (2)	O(3)—Cu—O(1ⁱⁱⁱ)	92·3 (2)

(b) In the phthalate anion

C(1)—C(2)	1·407 (9)	C(1)—C(7)	1·505 (9)
C(2)—C(3)	1·386 (10)	C(7)—O(1)	1·277 (8)
C(3)—C(4)	1·396 (10)	C(7)—O(2)	1·243 (8)
C(4)—C(5)	1·374 (12)	C(2)—C(8)	1·519 (10)
C(5)—C(6)	1·374 (10)	C(8)—O(3)	1·223 (8)
C(1)—C(6)	1·400 (10)	C(8)—O(4)	1·283 (8)
C(3)—H(1)	1·00 (7)	C(5)—H(3)	0·92 (7)
C(4)—H(2)	1·06 (9)	C(6)—H(4)	0·98 (7)

C(6)—C(1)—C(2)	119·0 (6)	C(4)—C(5)—C(6)	119·7 (7)
C(6)—C(1)—C(7)	117·4 (6)	C(1)—C(6)—C(5)	121·3 (7)
C(2)—C(1)—C(7)	123·6 (6)	C(1)—C(7)—O(1)	120·9 (6)
C(1)—C(2)—C(3)	119·1 (6)	C(1)—C(7)—O(2)	117·9 (6)
C(1)—C(2)—C(8)	126·1 (6)	O(1)—C(7)—O(2)	121·1 (6)
C(3)—C(2)—C(8)	114·8 (6)	C(2)—C(8)—O(4)	114·3 (6)
C(2)—C(3)—C(4)	120·7 (7)	C(2)—C(8)—O(3)	120·5 (6)
C(3)—C(4)—C(5)	120·3 (7)	O(4)—C(8)—O(3)	125·2 (6)
C(2)—C(3)—H(1)	124 (4)	C(4)—C(5)—H(3)	121 (4)
C(4)—C(3)—H(1)	116 (4)	C(6)—C(5)—H(3)	119 (4)
C(3)—C(4)—H(2)	121 (5)	C(5)—C(6)—H(4)	117 (4)
C(5)—C(4)—H(2)	117 (5)	C(1)—C(6)—H(4)	121 (4)

(c) Around the strontium cation

Sr—O(3)	2·618 (5)	Sr—O(2ⁱⁱⁱ)	2·643 (5)
Sr—O_w(2)	2·588 (6)	Sr—O_w(1ⁱᵛ)	2·549 (8)
Sr—O(1ⁱⁱⁱ)	2·773 (5)		

(d) In the water molecules

O_w(1)—H(5)	0·79 (8)	O_w(2)—H(6)	0·89 (9)
		O_w(2)—H(7)	0·78 (7)
H(5)—O_w(1)—H(5ⁱⁱ)	102 (9)	H(6)—O_w(2)—H(7)	113 (7)

(e) Hydrogen bonds

O_w(1)—H(5)···O(1)	3·032 (7)	O_w(1)—H(5)—O(1)	178 (9)
H(5)···O(1)	2·24 (8)	H(5)—O_w(1)—O(1)	1 (6)
O_w(2)—H(6)···O(2ⁱᵛ)	2·830 (8)	O_w(2)—H(6)—O(2ⁱᵛ)	159 (8)
H(6)···O(2ⁱᵛ)	1·98 (9)	H(6)—O_w(2)—O(2ⁱᵛ)	15 (6)
O_w(2)—H(7)···O(4ⁱ)	2·927 (7)	O_w(2)—H(7)—O(4ⁱ)	174 (7)
H(7)···O(4ⁱ)	2·15 (7)	H(7)—O_w(2)—O(4ⁱ)	5 (5)

Asymmetric units

(i)	x, −y, −½ + z	(iii)	−x, −y, −z
(ii)	−x, y, ½ − z	(iv)	x, −1 + y, z

All calculations were carried out on the CYBER 76 computer of the Centro di Calcolo Interuniversitario dell'Italia Nord-Orientale (Bologna).

Table 5. *Least-squares planes*

Equations of least-squares planes are in the form: $AX + BY + CZ = D$, where X, Y and Z are coordinates in Å referred to orthogonal axes obtained from fractional coordinates by applying the matrix: $(a, 0, c \cos \beta/0, b, 0/0, 0, c \sin \beta)$. Deviations (Å) of relevant atoms from the planes are in squares brackets.

	A	B	C	D
Plane (1): C(1)C(2)C(3)C(4)C(5)C(6)				
Compound (I)	−0·9771	−0·0461	−0·2076	−1·8314

[C(1) −0·013 (7), C(2) 0·008 (7), C(3) 0·008 (8), C(4) −0·019 (9), C(5) 0·008 (7), C(6) 0·009 (7), O(1) 0·325 (6), O(2) −0·844 (4), C(7) −0·212 (7), O(3) 1·241 (6), O(4) −0·779 (5), C(8) 0·148 (7)]

Compound (II)	0·2396	−0·7947	−0·5576	−1·5340

[C(1) −0·007 (6), C(2) 0·012 (7), C(3) −0·009 (8), C(4) −0·004 (9), C(5) 0·008 (8), C(6) −0·001 (8), O(1) 0·155 (5), O(2) −0·364 (5), C(7) −0·050 (6), O(3) 1·165 (5), O(4) −1·015 (5), C(8) 0·094 (6)]

Plane (2): C(1), C(7) O(1) O(2)				
Compound (I)	−0·7195	−0·3582	−0·5950	−4·8874

[C(1) −0·001 (6), C(7) 0·001 (6), O(1) −0·001 (5), O(2) −0·001 (4)]

Compound (II)	0·3745	−0·6309	−0·6795	−1·0145

[C(1) −0·009 (6), C(7) 0·021 (6), O(1) −0·005 (5), O(2) −0·006 (5)]

Plane (3): C(2)C(8)O(3)O(4)				
Compound (I)	−0·2686	0·6051	−0·7495	−1·6049

[C(2) −0·005 (6), C(8) −0·011 (6), O(3) 0·003 (4), O(4) 0·003 (5)]

Compound (II)	−0·4243	0·5973	−0·6806	−2·2448

[C(2) −0·010 (7), C(8) 0·021 (6), O(3) −0·006 (5), O(4) −0·005 (5)]

Discussion

Both structures (Figs. 1, 2) consist of linear polymeric chains, running along [001], of o-phthalatocuprate complexes, alkaline-earth cations and water molecules. Bond distances and angles are given in Table 3 for (I) and Table 4 for (II). In (I) the Cu atom, which lies on a binary axis, is surrounded in a square-planar arrangement by four O atoms belonging to four pht groups. Each pht group acts as a bridge through one O atom from each of its carboxylate groups. Cu also forms two longer contacts (2·851 Å) involving the uncoordinated O(4) atoms from two pht ions, so the coordination polyhedron assumes the form of a distorted octahedron (Fig. 3). In (II) the Cu atom, which lies on a centre of symmetry, is coordinated in an octahedral arrangement (Fig. 4) by six O atoms from four pht ions. Each pht anion bridges two adjacent Cu atoms in the usual way and chelates one of the two bridged Cu atoms. The distance between two bridged Cu atoms in (II) (Cu···Cu = 4·54 Å) is much shorter than that found in (I) (Cu···Cu = 6·83 Å) and in Li, K, Rb-o-phthalatocuprates (6·51, 5·74, 5·94 Å) (Cingi, Lanfredi, Tiripicchio & Camellini, 1977, 1978*b*). The least-squares planes and deviations of relevant atoms from them, for the two compounds (I) and (II), are given in Table 5. The carboxylate groups of pht are rotated with respect to the benzene ring, as usual on the same side in (I) [31° for C(1)C(7)O(1)O(2) and 67° for C(2)C(8)-O(3)O(4)] while in (II) they are rotated on opposite sides [14·1° for C(1)C(7)O(1)O(2) and −78·5° for C(2)C(8)O(3)O(4)] as found in the chelating pht (57

Table 6. *Conformation of the seven-membered coordination ring in the strontium compound*

Equation of least-squares plane through O(1)C(7)C(1)C(2)C(8) (see Table 5)

$$0.3191X - 0.7698Y - 0.5528Z = -1.2977$$

Displacements (Å) of relevant atoms from this plane

O(1) 0·029 (5), C(7) −0·070 (6), C(1) 0·044 (6), C(2) 0·019 (7), C(8) −0·022 (6), Cu 1·298 (1), O(3) 0·997 (5)

Torsion angles (°)

Cu–O(1)–C(7)–C(1)	57·9	C(2)–C(8)–O(3)–Cu	85·8
O(1)–C(7)–C(1)–C(2)	11·9	C(8)–O(3)–Cu–O(1)	−17·2
C(7)–C(1)–C(2)–C(8)	−4·7	O(3)–Cu–O(1)–C(7)	−64·9
C(1)–C(2)–C(8)–O(3)	−79·4		

and −50°) in BaCu^{II}pht$_2$.4H$_2$O (Cingi, Lanfredi, Tiripicchio & Camellini, 1978*c*). The double (chelating and bridging) behaviour of the pht ion in (II) is responsible for the closer approach of the doubly bridged Cu atoms in the chain and for the different values of the rotation angles of the carboxylate groups in the chelating pht. The bite distance [O(1)···O(3) = 3·04 Å] of the chelating group O(1)C(7)C(1)C(2)-C(8)O(3) in (II) is greater than the corresponding distance found in the Ba compound (2·72 Å). The data collected in Table 6 show that the conformation of the seven-membered coordination ring in (II) is envelope.

In (I) the Mg cation, which lies on a binary axis, is small enough to interpose between the chains and to
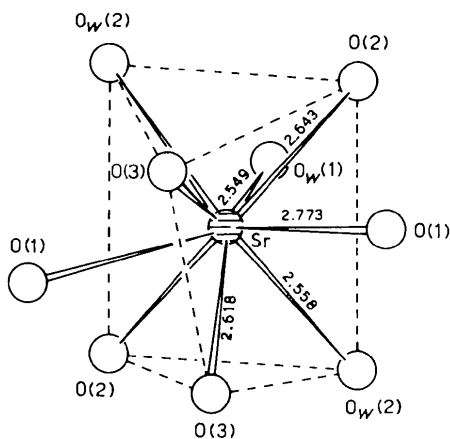
Fig. 5. Coordination around the Sr atom.

distorted trigonal prism (Fig. 5) with lateral centred faces. This type of coordination has been found in $Sr(IO_3)_2H_2O$ (Lanfredi, Pellinghelli, Tiripicchio & Camellini, 1972). The Sr—O interactions (Sr—O_{pht} 2·618–2·773; Sr—O_w 2·549–2·588 Å) together with hydrogen bonds between water molecules and O atoms of pht anions from adjacent chains, join the chains in layers parallel to (100). The packing of layers is determined by normal van der Waals contacts.

connect them in layers parallel to (010) by two bonds with two O atoms belonging to pht anions of adjacent chains. Coordination of Mg is completed to octahedral by four water molecules, which are important in packing because of the hydrogen bonds they form with carboxylate groups of adjacent chains. In (II) the Sr cation, which also lies on a binary axis, presents, because it is larger, more extensive coordination, being surrounded by six O atoms belonging to pht anions from the same chain and by three water molecules. The coordination around the Sr cation can be described as a

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